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MOVING LEAST SQUARES INTERPOLATION WITH THIN-PLATE SPLINES AND RADIAL BASIS FUNCTIONS

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Abstract—Moving least-squares methods for interpolation or approximation of scattered data are well known, and can suffer from defects, such as flat spots in the Shepard method, and edge effects inherited from a polynomial basis in the higher degree cases. We investigate methods based on thin-plate splines and on other radial basis functions. It turns out that a small support of the weight function leads to a small support for the "spline basis" and associated efficiency in the evaluation of the approximant. The edge effects seem minimal and good interpolants of scattered data can be obtained.

1. INTRODUCTION

Bivariate moving least-squares methods based on polynomials rely on the following principle. If $\mathbf{t}_i := (x_i, y_i)$, $i = 1, 2, \ldots, n$ are distinct points in the plane, not in the zero set of a polynomial of degree m satisfying $\binom{m+2}{2} < n$, and corresponding values $f_1, \ldots, f_n$ are given, the function-value at some point $\mathbf{t}^* := (x^*, y^*)$ is estimated as $g^*(\mathbf{t}^*)$, where $g^*(\mathbf{t})$ is a polynomial of degree m (usually low) in x and y which fits the given data in a weighted least-squares sense. Thus, g^* minimizes $\sum w_i^*[g(\mathbf{t}_i) - f_i]^2$, $g \in \mathcal{P}_m$, the linear space of bivariate polynomials of degree $\leq m$, and of dimension $\binom{m+2}{2}$. The weights are given by $w_i^* = w(\| \mathbf{t}^* - \mathbf{t}_i \|)$, where w is a non-negative weight function and $\| \cdot \|$ is the Euclidean distance. This process generates a surface which is, in general, not polynomial, depending as it does on the nature of the weight function.

An advantage of moving least-squares methods over some others, such as the thin-plate spline and other methods based on radial basis functions, is that it is possible to make them local by choosing w to have suitable compact support. On the other hand, moving least-squares methods with a polynomial basis tend to inherit the latter's disadvantages. Here, we will attempt to adapt the moving least-squares method to a radial basis, which is known to yield better interpolants.

It will be convenient to adopt the point of view that there is an underlying function $f(\mathbf{t})$, defined on a domain Ω containing the points $\mathbf{t}_i$, which is sampled in order to supply the data f_i. The moving least-squares (MLS) method can then be interpreted as an operator acting on f and generating a certain output. The operator based on polynomials, as described above, will be denoted PMLS, and we shall write PMLS(f) for the function obtained in this way. The spline-based method will be denoted SMLS. It is easy to see that PMLS(f) is a polynomial when the weight function w is constant. It is also shown by Lancaster and Šalkauskas [1] that if $f \in \mathcal{P}_m$ then PMLS(f) $= f$, and that PMLS is a projector from $\mathcal{C}(\Omega)$ into $\mathcal{C}^k(\Omega)$, the smoothness depending on that of w.

In general, PMLS(f) does not interpolate f because $\dim(\mathcal{P}_m) < n$. Interpolation can be achieved by choosing w to be unbounded at the origin. For example, the choice $w(r) = 1/r^2$ is a common one. The implications of such a singularity in w are discussed at length in [1], and we make use of it in Section 3. In the next two sections, we restrict ourselves to a case when $m = 1$; higher degree cases can be handled in a similar way and are discussed briefly in Section 4.

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2. A LEAST-SQUARES METHOD BASED ON THIN-PLATE SPLINES

We now turn to a least-squares method based on thin-plate splines. In Section 3 we modify it to an SMLS. An immediate problem with the construction of a moving method is that the basis functions for a thin-plate spline involve all of the translates of $r^2 \ln r$ to the data points, so that such a spline will interpolate and not have the moving aspect which can be used to create a local scheme by choosing a suitable weight function with compact support. However, the smoothing splines exploited by Wahba [2], Wahba and Wendelberger [3], and Wahba [4] (where other useful references will be found) minimize an energy functional combined with an "infidelity" functional in a convex way, and lead the way to the construction of an MLS method. We adapt this idea to our needs. For completeness, we include technical details which, for the most part, are fairly standard. We begin with the development of a weighted least-squares method based on thin-plate splines and exact for planar data. The resulting approximant is drawn from the Sobolev space

$$\mathcal{X} := \{u \in \mathcal{C}(\mathcal{R}^2) : D^m u \in \mathcal{L}_2(\mathcal{R}^2),\ |m| = 2\},$$

where m is a multi-index: $m := \{m_1, m_2\}$, $|m| := m_1 + m_2$, $D^m = \frac{\partial^{|m|}}{\partial x^{m_1}\,\partial y^{m_2}}$, and the derivatives are interpreted distributionally. The functional

$$F(u) := \sum_{|m|=2} \int_{\mathcal{R}^2} \binom{2}{m} [D^2 u(\mathbf{x})]^2 \, d\mathbf{x},$$

with $\binom{2}{m} = 2!/m_1!m_2!$ represents an approximation to the bending energy of u, and is a semi-norm for $\mathcal{X}$. It is now well known that there is a unique interpolating minimizer of $F(u)$—it is the thin-plate spline; see [5–7]. The principle of smoothing splines is to instead minimize the functional

$$S(u) := F(u) + (\mathbf{f} - \mathbf{u})^t W(\mathbf{f} - \mathbf{u}), \tag{1}$$

the bold facing indicating the evaluation of f and u at the $\mathbf{t}_i$, thus generating data vectors. Wahba [2] has considered this problem with $W = \alpha I$, α being a positive parameter. She has shown that the minimizer is a smoothing thin-plate spline. For $\alpha \to \infty$, the optimum is a thin-plate spline interpolant, for u is forced to reduce the second term to zero while minimizing the bending energy.

We now prepare an appropriate setting for an MLS method similar to the smoothing method above, by norming $\mathcal{X}$ and minimizing over $\mathcal{X}$ the functional defined by (1).

We note that $F(u)$ is derived from the semi-definite bilinear functional

$$A(u,v) := \sum_{|m|=2} \int_{\mathcal{R}^2} \binom{2}{m} D^2 u(\mathbf{x})\, D^2 v(\mathbf{x}) \, d\mathbf{x}, \tag{2}$$

which vanishes on $\mathcal{P}_1 \times \mathcal{P}_1$. In order to construct a norm for $\mathcal{X}$, we define a least-squares projector $P : \mathcal{X} \to \mathcal{P}_1$ by choosing a symmetric positive definite matrix $W \in \mathcal{R}^{n\times n}$ and putting Pu equal to a weighted least squares approximation to u from $\mathcal{P}_1$. Thus, Pu minimizes $\sum_{i=1}^n w_i[(Pu)(\mathbf{t}_i) - u(\mathbf{t}_i)]^2$ for some positive weights w_i. Writing $(Pu)(\mathbf{t}) = a_0 + a_1 x + a_2 y$, one finds that $\mathbf{a}^t = (a_0, a_1, a_2)$ satisfies the usual normal equations, whence $(Pu)(\mathbf{t}) = (1, \mathbf{t})\mathbf{a}$ has the form [8, Sec. 10.2]

$$(Pu)(\mathbf{t}) := (1, \mathbf{t})(VWV^t)^{-1}\, VW u,$$

where $\mathbf{u}^t := (u_1, \ldots, u_n)$, $u_i = u(\mathbf{t}_i)$ and

$$V = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ x_1 & x_2 & \cdots & x_n \\ y_1 & y_2 & \cdots & y_n \end{bmatrix}. \tag{3}$$

Our assumption about the data means that V has full rank. Now define the bilinear functional $B : \mathcal{X} \times \mathcal{X} \to \mathcal{R}$ by

$$B(u,v) := (\mathbf{Pu})^t W(\mathbf{Pv}), \tag{4}$$

the bold-facing indicating that the function Pu is evaluated at the data-points, thus generating a data vector.

We may now decompose $\mathcal{X}$ into a direct sum $\mathcal{X}_0 \oplus \mathcal{P}_1$ by means of the projector P, and note that the bilinear functional $N := A+B$ is an inner-product for $\mathcal{X}$. It is easy to see that $\mathcal{X}_0$ and $\mathcal{P}_1$ are mutually orthogonal in this inner-product, for if $u_0 \in \mathcal{X}_0$ and $u_1 \in \mathcal{P}_1$, then $A(u_0, u_1)$ clearly vanishes, and, since $u_0 = v - Pv$ for some $v \in \mathcal{X}$ and P is a projector, $Pu_0 = Pv - P^2v = 0$, so $B(u_0, u_1) = 0$ as well. Further, if we write $u \in \mathcal{X}$ as $u = u_0 + u_1$, where $u_0 = u - Pu \in \mathcal{X}_0$ and $u_1 = Pu \in \mathcal{P}_1$, then $N(u, u) = F(u_0) + B(u_1, u_1)$. The square root of the first term F defines a norm $\|\cdot\|_0$ for $\mathcal{X}_0$, while the square root of the second yields a norm $\|\cdot\|_1$ for $\mathcal{P}_1$ since $n > 3$.

The optimization problem that we now consider is to determine $g^* \in \mathcal{X}$ which approximates f by minimizing $S(u)$ (equation (1)).

Applying P to u and f in order to get their components in X_0 and $\mathcal{P}_1$, we find (with the same bold-face notation for vectors as before) that

$$S(u) = \|u_0\|_0^2 + (\mathbf{u}_0 - \mathbf{f}_0)^t W(\mathbf{u}_0 - \mathbf{f}_0) + \|\mathbf{u}_1 - \mathbf{f}_1\|_1^2 , \tag{5}$$

because the terms $(\mathbf{u}_0 - \mathbf{f}_0)^t W(\mathbf{u}_1 - \mathbf{f}_1)$ and $(\mathbf{u}_1 - \mathbf{f}_1)^t W(\mathbf{u}_0 - \mathbf{f}_0)$ vanish. This follows from a simple calculation which uses the fact that $\mathbf{Pv} = V^t(VWV^t)^{-1} VW\mathbf{v}$.

The minimization of $S(u)$ thus falls into two parts; we may immediately choose $u_1 = f_1 = Pf$. To minimize the portion involving u_0, we make use of the fact, shown e.g., by Duchon [5] and Meinguet [6], that $\mathcal{X}_0$ is a Hilbert space in which the evaluation functional δ_{t_k} has a representer g_k. Taking the representers $g_1, g_2, \ldots, g_n$, we find that a subset of $n-3$ of them is linearly independent. Without loss of generality, we may assume that this set is $\{g_k\}_1^{n-3}$ (details of this are made explicit following (7)). This set can be orthonormalized to $\{\tilde{g}_k\}_1^{n-3}$ by the Gram-Schmidt process, and extended to a complete orthonormal basis $\{\tilde{g}_k\}_1^\infty$ for $\mathcal{X}_0$. Putting $u_0 = \sum_1^\infty a_k \tilde{g}_k$, we have $a_k = A(u_0, \tilde{g}_k)$, and $\|u_0\|_0^2 = \sum_1^\infty a_k^2$. Since $u_0(\mathbf{t}_i) = A(u_0, g_i)$, it follows from orthogonality that $u_0(\mathbf{t}_i)$, and hence the middle term of (5), only involves the first $n-3$ g_k's. Consequently, the sum of the first two terms of $S(u)$ in (5) can be reduced in magnitude by choosing $a_k = 0$ for $k \geq n-2$. It follows that $u_0 \in \operatorname{span}\{g_k\}_1^{n-3}$.

We postpone the calculation of the explicit form of the representers and proceed with the minimization. Put $u_0 = \sum_1^{n-3} b_k g_k$; then $|u_0|_0^2 = \mathbf{b}^t\mathrm{G}\mathbf{b}$, with $\mathrm{G} := [g_i(\mathbf{t}_j)] \in \mathcal{R}^{(n-3)\times(n-3)}$, and $b \in \mathcal{R}^{n-3}$, because the g_k's are representers. But $g_i(t_j) = A(g_i, g_j) = A(g_j, g_i) = g_j(\mathbf{t}_i)$, so G is symmetric (as is W), and a Gram matrix of linearly independent functions, hence positive definite. We next show that the middle term of (5) can be written in the form

$$(\mathbf{u}_0 - \mathbf{f}_0)^t W(\mathbf{u}_0 - \mathbf{f}_0) = (\mathbf{b}^t G - \mathbf{w}_0^t) Z(G\mathbf{b} - \mathbf{w}_0),$$

where $\mathbf{w}_0$ is the vector of the first $n-3$ components of $\mathbf{f}_0$, and Z is a certain positive definite matrix. To see this, assume that the given data points are arranged so that the last three form a $\mathcal{P}_1$-unisolvent set. Then we may partition the matrix V of (3) into $[V_1, V_2]$, where V_2 is a non-singular 3×3 matrix. Also, we partition W into $\operatorname{diag}[W_1, W_2]$, with $W_1 \in \mathcal{R}^{(n-3)\times(n-3)}$ and $W_2 \in \mathcal{R}^{3\times 3}$. For any $u_0 \in \mathcal{X}_0$ write $\mathbf{u}_0^t = (\mathbf{u}^t, \mathbf{v}^t)$ with $\mathbf{u} \in \mathcal{R}^{n-3}$, $v \in \mathcal{R}^3$, and abbreviate $L := (VWV^t)^{-1}$. Now, $\mathbf{u}_0 \in \mathcal{X}_0$ implies $P\mathbf{u}_0 = 0$, from which we have

$$(1, x, y)\, L(V_1 W_1 \mathbf{u} + V_2 W_2 \mathbf{v}) = 0$$

identically in x and y. Evaluating this at $(x, y) = \mathbf{t}_k$, $\mathbf{k} = n-2,\ n-1,\ n$, we obtain a system which can be solved for $\mathbf{v}$, and yields

$$\mathbf{v} = -W_2^{-1} V_2^{-1} V_1 W_1 \mathbf{u}. \tag{6}$$

Define

$$U_2 := -W_2^{-1} V_2^{-1} V_1 W_1 \in \mathcal{R}^{3\times(n-3)}, \quad U := [I_{(n-3)\times(n-3)}, U_2^t]^t \in \mathcal{R}^{n\times(n-3)},$$
$$Z := U^t W U. \tag{7}$$

Equation (6) shows that the representers g_k, $k = n-2$, $n-1$, n are linear combinations of $g_1, \dots, g_{n-3}$. Now it is easy to see that since $\mathbf{u}_0 = G\mathbf{b}$, the middle term of (5) can be written in the form

$$(\mathbf{b}^t G - \mathbf{w}_0^t)\, Z(G\mathbf{b} - \mathbf{w}_0),$$

so we are to minimize the positive definite quadratic form

$$\mathbf{b}^t(G + GZG)\,\mathbf{b} - 2\mathbf{b}^t\, GZ\mathbf{w}_0 + \mathbf{w}_0^t\, Z\mathbf{w}_0.$$

Differentiating with respect to $\mathbf{b}$ we get the condition for a minimum:

$$[(G + GZG)^t + (G + GZG)]\,\mathbf{b} - 2GZ\mathbf{w}_0 = 0.$$

By symmetry of Z and G this simplifies and yields

$$\mathbf{b} = (I + ZG)^{-1} Z\mathbf{w}_0.$$

Thus, the complete optimizer is

$$\begin{aligned} g^* &= (g_1, g_2, \dots, g_{n-3})(I + ZG)^{-1}\, Z\mathbf{w}_0 + Pf \\ &= (g_1, g_2, \dots, g_{n-3})(Z^{-1} + G)^{-1}\,\mathbf{w}_0 + Pf. \end{aligned} \tag{8}$$

We now compute the representers. Since A is the inner product for $\mathcal{X}_0$ (see equation (2)), a representer of function evaluation, say g_k, satisfies $A(g_k, u) = u(\mathbf{t}_k)$ for all $u \in \mathcal{X}_0$. Letting $\mathcal{D}$ be the usual space of C^∞ test functions with compact support in $\mathcal{R}^2$, clearly $\varphi - P\varphi \in \mathcal{X}_0$, and, following Meinguet [6], representers can be found by first solving the distributional differential equation $A(E, \varphi - P\varphi) = \varphi(0)$, for $\varphi \in \mathcal{D}$. It is found that, for a certain constant c and $r = \|\,\mathbf{t}\,\|_2$, $E(\mathbf{t}) := cr^2 \ln r$ solves the equation above. Now the restriction of the point evaluation functional $\delta_\mathbf{u}$ to $\mathcal{X}_0$ is represented by

$$\langle \delta_\mathbf{u}, \varphi - P\varphi\rangle = \langle \delta_\mathbf{u}, \varphi\rangle - \sum_{i=1}^{n} p_i(\mathbf{u})\, \varphi(\mathbf{t}_i) = \langle \delta_\mathbf{u}, \varphi\rangle - \sum_{i=1}^{n} p_i(\mathbf{u}) \langle \delta_{\mathbf{t}_i}, \varphi\rangle,$$

where $\langle d, \varphi\rangle = d(\varphi)$ for a distribution d, and we have defined

$$\mathbf{p}^t(\mathbf{t}) = (p_1(\mathbf{t}), p_2(\mathbf{t}), \dots, p_n(\mathbf{t})) := (1, \mathbf{t})(VWV^t)^{-1}\, VW. \tag{9}$$

Since $v - Pv = 0$ for all $v \in \mathcal{P}_1$, the distribution

$$\mu := \delta_\mathbf{u} - \sum_{i=1}^{n} p_i(\mathbf{u})\, \delta_{\mathbf{t}_i}$$

is, in the terminology of Meinguet [7], an evaluation linear functional with finite support in $\mathcal{R}^2$, annihilating $\mathcal{P}_1$. By Theorem 2 of Meinguet [7], the convolution $H_\mathbf{u}(\mathbf{t}) := \mu * E(\mathbf{t}) \in \mathcal{X}$, and hence $h_\mathbf{u}(\mathbf{t}) := (I - P)\, H_\mathbf{u}(\mathbf{t}) \in \mathcal{X}_0$ is the representer of function evaluation at $\mathbf{u}$. Explicitly, for $\mathbf{u} = \mathbf{t}_i$, $i = 1, 2, \dots, n$,

$$\begin{aligned} g_i(\mathbf{t}) := h_{\mathbf{t}_i}(\mathbf{t}) &= E(\mathbf{t} - \mathbf{t}_i) - \sum_{j=1}^{n} p_j(\mathbf{t}_i)\, E(\mathbf{t} - \mathbf{t}_j) \\ &\quad - \sum_{j=1}^{n} p_j(\mathbf{t})\, E(\mathbf{t}_j - \mathbf{t}_i) + \sum_{j=1}^{n}\sum_{k=1}^{n} p_j(\mathbf{t})\, p_k(\mathbf{t}_i)\, E(\mathbf{t}_j - \mathbf{t}_k). \end{aligned} \tag{10}$$

Here, $E(\mathbf{s} - \mathbf{t}) = c\|\mathbf{s} - \mathbf{t}\|^2 \ln \|\mathbf{s} - \mathbf{t}\|$, $c := 1/(8\pi)$, and the p_j's are as in (9). Equation (8) displays g^* in a Boolean sum form $(Q \oplus P)f$. Here, P is the projector of (3), and $Q : \mathcal{X}_0 \to \operatorname{span}\{g_k\}_1^{n-3}$ is not a projector. However, if $W = \alpha I$, then as $\alpha \to \infty$, Q becomes an interpolating projector and the limiting g^* is an interpolating thin-plate spline. In the moving context, P is position-dependent, and $Pf = \text{PMLS}(f)$, i.e., an interpolant if a singular weight function is used.

3. AN SMLS METHOD

We now convert the least-squares method of the preceding section into an SMLS method by proceeding as in the PMLS case and using a position-dependent weight matrix W. As described in Section 1, a point of evaluation $\mathbf{t}^*$ of the least-squares approximant is fixed during the calculation of MLS(f), so that W, the projector $\mathcal{P}$ and the associated spline basis of representers g_k depend on $\mathbf{t}^*$. W will be diagonal, and for consistency it will be normalized so that trace $(W) = 1$. It is not clear at this point whether this is the best normalization for a moving method. To permit varying amounts of influence for the second term of the functional (1), we shall then replace W by λW. The only quantity affected by this is the matrix Z of (7), and so we replace Z by λZ in (7) and (8). The degree of differentiability of the elements of the W matrix directly affects that of SMLS(f), and since $r^2 \ln r$ is C^∞ except at the origin, where it is C^1, a twice differentiable W will yield SMLS(f) $\in C^2(\Omega\backslash\{\mathbf{t}_i\})$. If SMLS is to interpolate, a singularity has to be introduced in the weight function. In particular, the choice $w(r) = m(r)\, r^{-\alpha}$, for non-negative $m(r) \in C^2(\Omega)$ and even $\alpha > 0$, yields a twice differentiable Pf by an analysis similar to that in [1].

Now let P be the Vandermondian obtained from (9) by defining

$$P := WV^t(VWV^t)^{-1}\, V \tag{11}$$

(we do not distinguish between the projector P onto $\mathcal{P}_1$ and its matrix representation). It is then not hard to see that (see (9),(10)) the vector of representers and their Vandermondian can be written in the forms

$$g(\mathbf{t}) = \mathbf{E}(\mathbf{t}) - P^t\, \mathbf{E}(\mathbf{t}) - E\mathbf{p}(\mathbf{t}) + P^t E\mathbf{p}(\mathbf{t}), \qquad G^* = E - P^t E - EP + P^t EP, \tag{12}$$

respectively, where $\mathbf{E}(\mathbf{t})$ is the column vector of translates of $E(\mathbf{t})$ and E is the (symmetric) $n \times n$ Vandermondian $[E(\mathbf{t}_i - \mathbf{t}_j)]$. The matrix G of (8) is the $(n-3) \times\ (n-3)$ upper left-hand corner of G^*. In computations, care must be exercised to remove the indeterminacy when $\mathbf{t}$ is near $\mathbf{t}_i$. By choosing a weight function with sufficiently large compact support, it is possible to localize the computation of SMLS(f). Suppose, then, that $w : [0, R) \to \mathcal{R}^+$ is a C^2 weight function with support $[0, R]$. Let $\mathbf{t}^* \in \Omega$ be fixed, and take for W the diagonal weight matrix with elements $w^*_{ii}\ :=\ w(\|\mathbf{t}^* - \mathbf{t}_i\|)$. If R is sufficiently large, then the disk $\|\mathbf{t}^* - \mathbf{t}\| < R$ will contain a set of points $\{\mathbf{t}_i\}_{i \in I}$, containing in turn a $\mathcal{P}_1$-unisolvent triple of points, so that the projector P is well-defined. A number of weights in the weight matrix W can be expected to vanish. As a result, the optimization problem obtains a block structure with some zero blocks; this is reflected in the solution g^* involving fewer than $n-3$ g_k's and some economies in the computation. This means that while the global (at least on Ω) cardinal basis for this interpolation method has not been explicitly constructed, and depends in a quite complicated way on the spline basis $\{g_k\}_0^{n-3}$, it is compactly supported. We then take SMLS(f)($\mathbf{t}^*$) $= g^*(\mathbf{t}^*)$. If R is large, the computational effort can be prohibitive, for g^* has to be computed anew for each point at which the interpolating surface is to be evaluated. However, the idea lends itself to parallel implementation and to local interpolated refinement of the given data set. Also, SMLS(f) can be used to supply nodal values for another local interpolant, such as Clough-Tocher, especially since its derivatives are easily evaluated.

The results of some computational experiments are shown in the figures. Figure 1 shows a ramp-mountain function which is only C^0 and can be expected to cause difficulties. The location of the date points is shown in the scatterplot of Figure 2. We have some previous experience with interpolation of this function by various methods; results can be found in [8]. Only 40 data points are used in Figures 3–8. The thin plate spline shown in Figure 3 for this data is very smooth but sluggish with substantial undulations. Figures 4–6 show SMLS(f)'s using $w(r) = (R-r)^2/r^4$ with $R = 3$ and various values of λ. With this value of R, the supports of the translates of $w(r)$ contain all of the domain of f. For the smaller values of λ there is little difference—that can be seen in this kind of picture, between the PMLS(f) $= Pf$ shown in Figure 7 and the SMLS(f)'s. As λ increases, the surface becomes more spline-like and looks less like the model surface. It should be recalled, however, that unlike usual thin-plate spline interpolation, this method can be local for a suitable choice of $w(r)$.

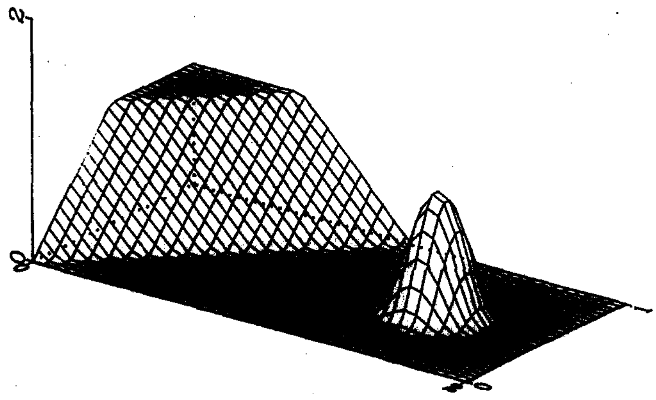

Figure 1. Model problem.

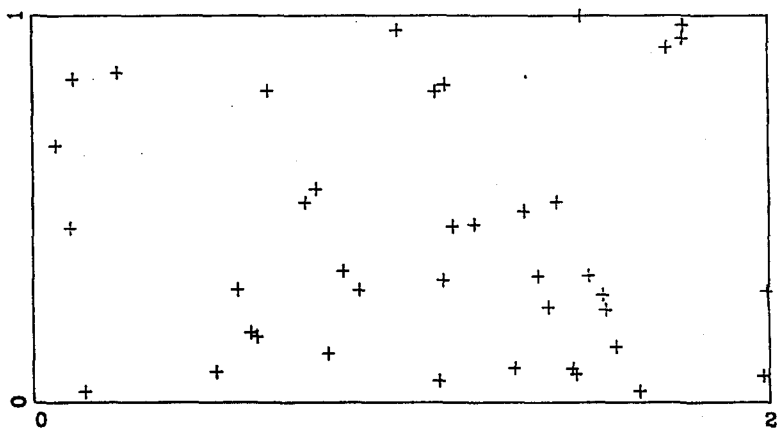

Figure 2. Scatter plot.

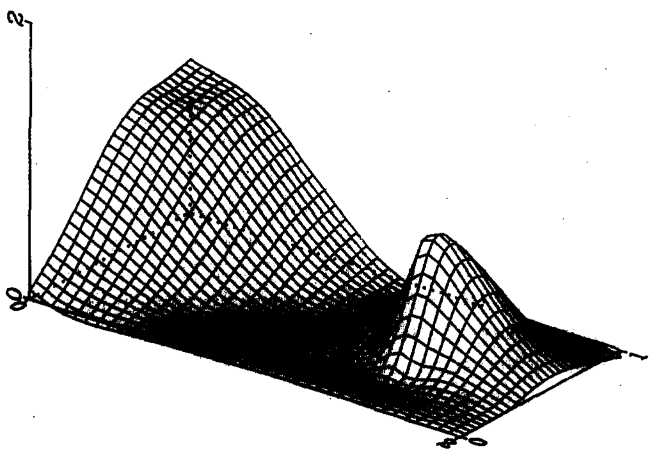

Figure 3. Thin-plate spline.

4. OTHER MLS METHODS

The method developed above can be generalized by working with the family of spaces and seminorms considered by, for example, Meinguet [6] and Wahba [2]. Thus, let $\mathcal{D}$ be the space of C^∞ functions with compact support in $\mathcal{R}^N$ and take for $\mathcal{X}$ the space of all distributions on $\mathcal{D}$ whose derivatives of total order m are square integrable over $\mathcal{R}^N$. A seminorm is then defined for $\mathcal{X}$ by

$$| u |_m^2 := \int_{\mathcal{R}^N} \sum_{i_1,\ldots,i_m}^{N} \left[\frac{\partial^m u}{\partial x_{i_1} \ldots \partial x_{i_m}} \right]^2 dx.$$

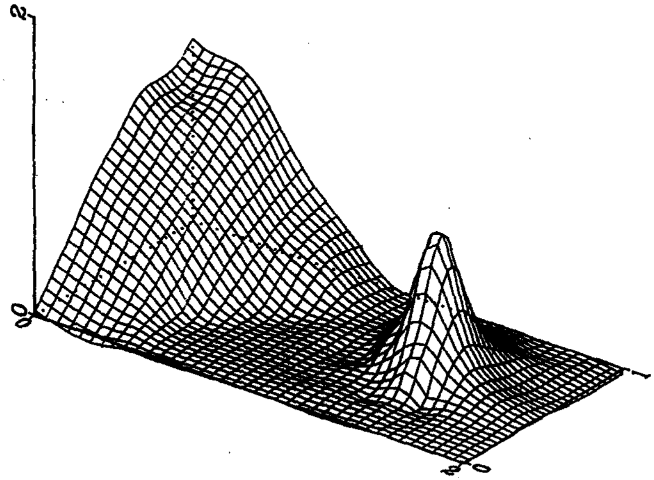

Figure 4. Spline MLS ($\lambda = 1$).

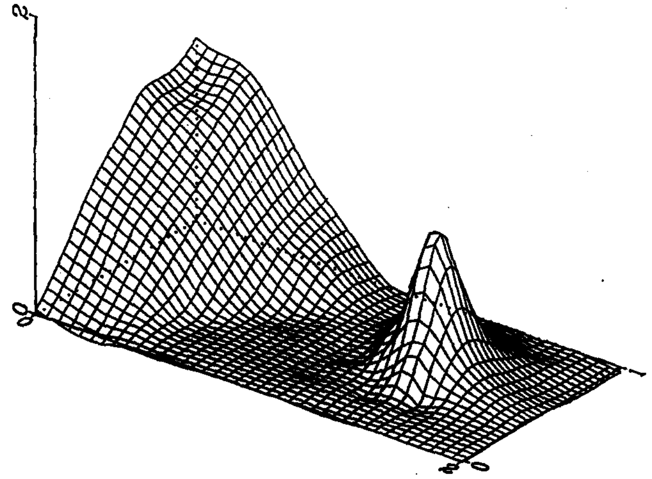

Figure 5. Spline MLS ($\lambda = 100$).

If $m > N/2$, $\mathcal{X}$ is a space of continuous functions, and the kernel of $|\cdot|_m$ is $\mathcal{P}_{m-1}$. We have dealt only with the case $N = m = 2$. In the more general setting, adjustments have to be made to the projector P so that it maps $\mathcal{X}$ onto $\mathcal{P}_{m-1}$, and the fundamental solution from which the representers are calculated is

$$E(\mathbf{t}) = \begin{cases} c\, r^{2m-N} \ln r, & N \text{ even}, \\ d\, r^{2m-N}, & N \text{ odd}, \end{cases}$$

and

$$c = \frac{(-1)^{1+2/N}}{2^{2m-1}\, \pi^{N/2}(m-1)!(m-N/2)!},$$
$$d = \frac{(-1)^m\, \Gamma(N/(2-m))}{2^{2m}\, \pi^{N/2}(m-1)!}.$$

Details concerning the theoretical basis for this can be found in [6,8].

Other methods can be obtained as a result of the observation that SMLS is completely determined by the projector P (and hence W) and the radially symmetric function $E(\mathbf{t})$. The functions $E(\mathbf{t})$ defined above not only generate representers, but are also conditionally positive definite of order m in the following sense. Let $\{b_i\}_1^M$ be a basis for $\mathcal{P}_{m-1}$, the space of polynomials of degree $\leq m-1$ on $\mathcal{R}^N$, which has dimension $M = \binom{N+m-1}{N}$, and let V be, as before, the $M \times n$ matrix with elements $b_i(\mathbf{t}_j)$. Let $E(\mathbf{t})$ be a continuous function defined on $\mathcal{R}^N$ and let E

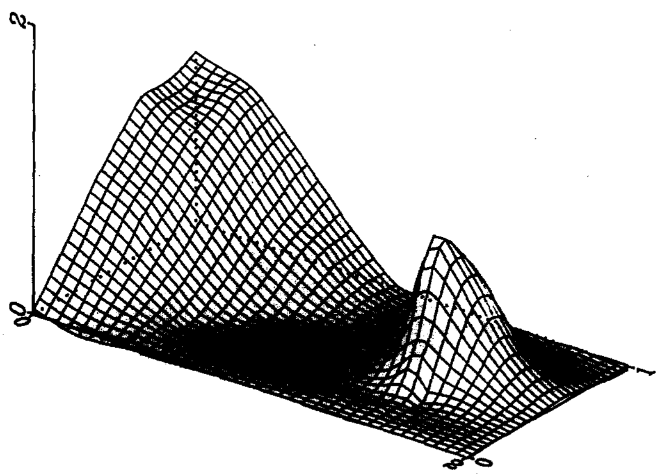

Figure 6. Spline MLS ($\lambda = 10000$).

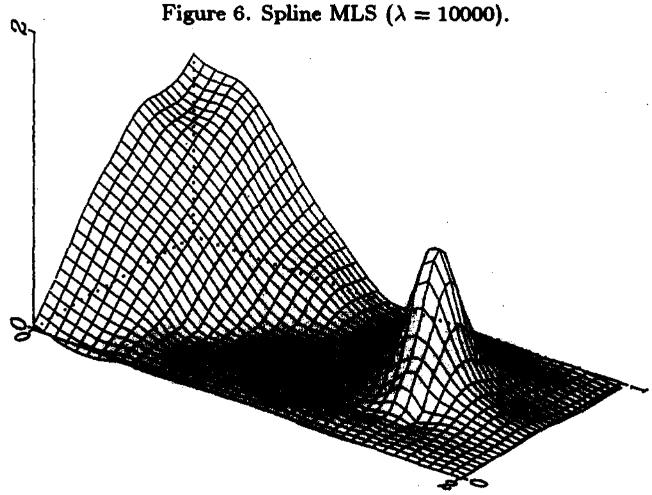

Figure 7. PMLS interpolant.

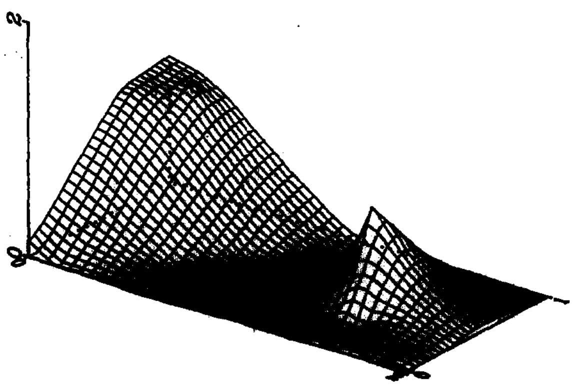

Figure 8. Multiquadric interpolant ($c = 0.01$).

be the associated distance matrix $[E(\mathbf{t}_i - \mathbf{t}_j)] \in \mathcal{R}^{n\times n}$. This symmetric matrix is, of course, the Vandermondian of the translates of the $E(\mathbf{t})$. $E(\mathbf{t})$ is said to be conditionally positive definite of order m if $\mathbf{u}^t E \mathbf{u} \geq 0$ for any $\mathbf{u}$ such that $V\mathbf{u} = 0$ and for any set of distinct points $\{\mathbf{t}_i\}_1^n$. If $E(\mathbf{t})$ is conditionally positive definite of order m, then the matrix G^* of (12) is singular, but its principal $(n-M)\times(n-M)$ submatrix G is conditionally definite provided that the points $\mathbf{t}_{n-M+1},\ldots,\mathbf{t}_n$ are not in the zero set of a polynomial in $\mathcal{P}_{m-1}$. To see this, note that $\dim[Im(P)] = M$ and $P^2 = P$ imply that $Im(P)$ contains a non-zero vector $\mathbf{x}$ and $P\mathbf{x} = \mathbf{x}$, so that $\lambda = 1$ is an eigenvalue of P. Hence, since $G^* = (I - P^t)\,E(I - P)$, $\det G* = 0$. On the other hand, suppose

$0 \neq x \in \mathcal{R}^{n-M}$, and put $\mathbf{y}^t = (\mathbf{x}^t, 0) \in \mathcal{R}^n$. By the zero set assumption above, $\mathbf{y} \notin Im(P)$ so that $\mathbf{u} := (I - P)\mathbf{y} \neq 0$. However, $V\mathbf{u} = 0$ (see (11)), and so $\mathbf{x}^t G\mathbf{x} = \mathbf{y}^t G^* \mathbf{y} = \mathbf{u}^t E\mathbf{u} \geq 0$.

If $E(\mathbf{t})$ is a conditionally positive definite function which generates representers of function evaluation with respect to some inner-product, then the associated optimization problem fits into a theory analogous to that of Section 2. If such an inner product is not available but the matrix E is strictly conditionally positive definite, then we may proceed formally as before, noting that equation (6) also continues to hold, *mutatis mutandis*. The limiting form of g^* as $\lambda \to \infty$ is (recall that Z in (8) is replaced by λZ)

$$g^* = (g_1, g_2, \ldots, g_{n-M})G^{-1}\mathbf{w}_0 + Pf.$$

Since $(g_1, g_2, \ldots, g_{n-M})G^{-1}$ is a vector of cardinal functions, the first term in g^* interpolates the data $\mathbf{w}_0$, which is the first $n - M$ components of the residual $f - Pf$. By virtue of (6), g^* interpolates all of the data. It should be noted that the presence of W in the various parts of g^* means that g^* need not coincide with the usual thin-plate spline.

A source of suitable $E(\mathbf{t})$'s is in the work of Micchelli [9]. It is shown there, for example, that $E(\mathbf{t}) := (r^2 + c^2)^{k-a}, r = \|\mathbf{t}\|$, the basis of the Hardy multiquadric method, is conditionally strictly positive definite of order k for $0 < a < 1$, for any n. The choice $k = 1$ and $a = 1/2$ thus yields a multiquadric method in an MLS form, and we use a projector P onto $\mathcal{P}_0$. Consequently, Pf is Shepard's method. Numerical experiments with this interpolant were quite unsuccessful. With increasing λ, extreme oscillations occur. The reasons for this are not clear at this time. The standard multiquadric is shown in Figure 8 and is reasonable, though not as good as any of the previous figures with a spline basis. In [8], an example of a badly oscillatory multiquadric also occurs; there, the size of the parameter c (see above) seems critical. Some more development of a theoretical basis for the use of these and other radial functions in the MLS context seems to be called for.

REFERENCES

1. P. Lancaster and K. Šalkauskas, Surfaces generated by moving least squares methods, *Math. Comp.* **37** (155), 141–158 (1981).
2. G. Wahba, Spline bases, regularization, and generalized cross validation for solving approximation problems with large quantities of noisy data, In *Approximation Theory III*, pp. 905–912, Academic Press, New York, (1980).
3. G. Wahba and J. Wendelberger, Some new mathematical methods for variational objective analysis using splines and cross validation, *Monthly Weather Review* **108** (8), 36–57 (1980).
4. G. Wahba, Spline models for observational data, In *Series in Applied Mathematics*, Vol. 59, SIAM, (1990).
5. J. Duchon, Splines minimizing rotation-invariant semi-norms in Sobolev spaces, In *Constructive Theory of Functions of Several Variables*, (Edited by W. Schempp and K. Zeller), pp. 85–100, Springer-Verlag, (1977).
6. J. Meinguet, Multivariate interpolation at arbitrary points made simple, Rapport No. 118, Presented at the *Seminaire de Mathématique Appliquée*, Institut de Mathématique Pure et Appliquée, Université Catholique de Louvain, Louvain-La-Neuve, (1978).
7. J. Meinguet, An intrinsic approach to multivariate spline interpolation at arbitrary points, In *Proceedings of the NATO Advanced Study Institute on Polynomial and Spline Approximation*, (Edited by B.N. Sahney), pp. 163–190, Reidel, Calgary, (1979).
8. P. Lancaster and K. Šalkauskas, *Curve and Surface Fitting; An Introduction*, Academic Press, London, (1986).
9. C.A. Micchelli, Interpolation of scattered data: Distance matrices and conditionally positive definite functions, *Constr. Approx.* **2** (1), 11–22 (1986).